

o-Allyl oo-tert-butylsuccinate

Inchi:	InChI=1S/C11H18O5/c1-5-8-14-9(12)6-7-10(13)15-16-11(2,3)4/h5H,1,6-8H2,2-4H3
InchiKey:	QPPROZHNOJODIC-UHFFFAOYSA-N
Formula:	C11H18O5
SMILES:	<chem>C=CCOC(=O)CCC(=O)OOC(C)(C)C</chem>
Mol. weight [g/mol]:	230.26
CAS:	52345-52-5

Physical Properties

Property code	Value	Unit	Source
gf	-440.42	kJ/mol	Joback Method
hf	-775.51	kJ/mol	Joback Method
hfl	-817.00 ± 4.00	kJ/mol	NIST Webbook
hfus	22.31	kJ/mol	Joback Method
hvap	58.84	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.769		Crippen Method
mcvol	182.300	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
tb	619.53	K	Joback Method
tc	809.17	K	Joback Method
tf	380.94	K	Joback Method
vc	0.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.03	J/mol×K	619.53	Joback Method
cpg	534.78	J/mol×K	777.56	Joback Method
cpg	523.80	J/mol×K	745.95	Joback Method
cpg	512.14	J/mol×K	714.35	Joback Method
cpg	499.79	J/mol×K	682.74	Joback Method
cpg	486.76	J/mol×K	651.14	Joback Method
cpg	545.09	J/mol×K	809.17	Joback Method
dvisc	0.0001226	Paxs	619.53	Joback Method

dvisc	0.0001595	Paxs	579.76	Joback Method
dvisc	0.0002158	Paxs	540.00	Joback Method
dvisc	0.0003064	Paxs	500.24	Joback Method
dvisc	0.0004621	Paxs	460.47	Joback Method
dvisc	0.0007533	Paxs	420.70	Joback Method
dvisc	0.0013597	Paxs	380.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52345525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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